Supporting information for article:

Coordination polymers of Cd[II] and Pb[II] with croconate show remarkable differences in coordination patterns: a structural and spectroscopic study

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1. UV-Vis titrations:

The binding curves for titrations of $Na_2C_5O_5$ with $Pb(NO_3)_2$ or $Cd(NO_3)_2 \cdot 4H_2O$ in 1:1 water:ethanol are shown in Figures S1 and S2. The binding constant for 1-1 complex formation was determined by non-linear regression analysis of the 1-1 binding isotherm. The data were fitted according to the 1-1 binding isotherm (Eq. 1) using non-linear regression methods:

$$\Delta A = A_{obs} - A_{init} = -([R]_t + [M]_t + K_{11}^{-1} - ((([R]_t + [M]_t + K_{11}^{-1})^2 - 4[M]_t [R]_t)^{1/2})) \Delta A_{max} / (2[R]_t) \ (Eq.1)$$

in which, K_{11} is the binding constant for 1-1 complex formation, $[R]_t$ is the constant concentration of rhodizonate in the solution, and $[M]_t$ is the variable concentration of added metal salt.
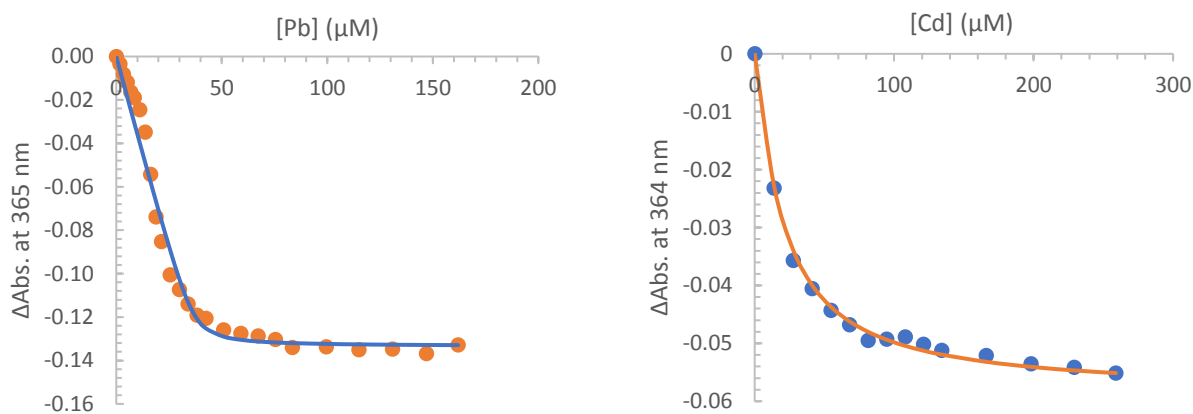

Figure S1 (left): Binding curve for the titration of a solution of 3.66 x 10^{-5} M of $Na_2C_5O_5$ with solution of 2.50 x 10^{-3} M of $Pb(NO_3)_2$ in 3.66 x 10^{-5} M of $Na_2C_5O_5$ in 1:1 water:ethanol. K_{11} = 1.85 x 10^6 M^{-1}.
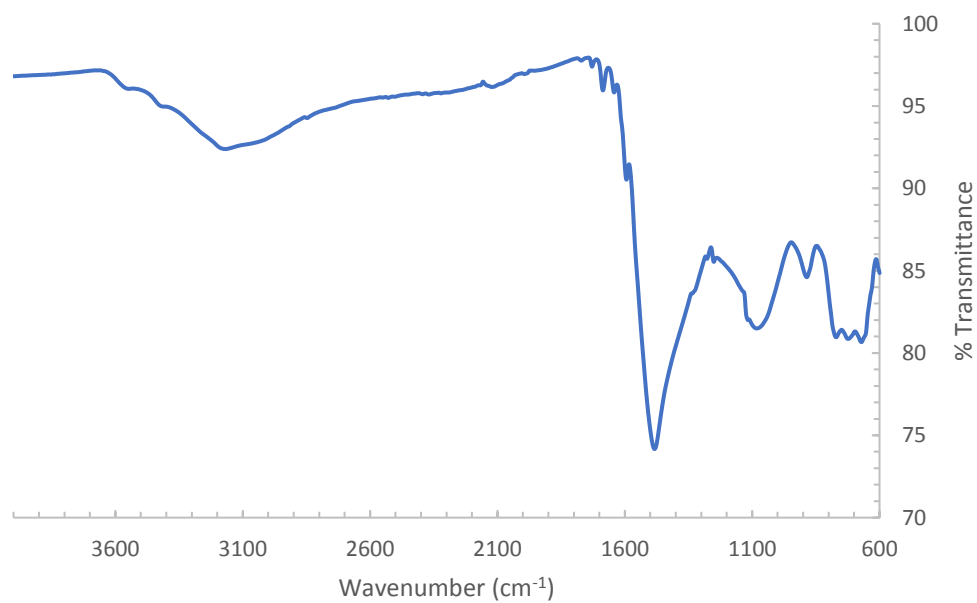
Figure S2 (right): Binding curve for the titration of a solution of 3.12 x 10^{-5} M of $Na_2C_5O_5$ with 8.29 x 10^{-3} M of $Cd(NO_3)_2 \cdot 4H_2O$ in 3.12 x 10^{-5} M of $Na_2C_5O_5$ in 1:1 water:ethanol. K_{11} = 1.30 x 10^5 M^{-1}.

2. FT-IR Spectroscopy

The IR spectra for the PbCroc and CdCroc complexes are shown in Figures S3 and S4, respectively.
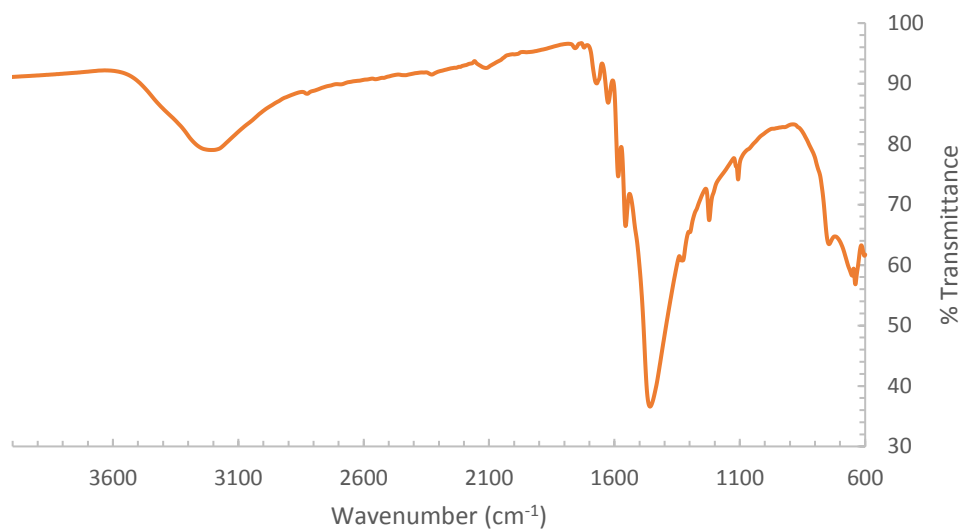
Figure S3: FT-IR spectrum of the PbCroc complex.

Figure S4: FT-IR spectrum of the CdCroc complex.